6/3/05 10/091,447

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

Structure search
3 hits CAPLUS
Co-pending apps
Tetrahedron letter article by inventor

FILE 'HOME' ENTERED AT 11:20:35 ON 03 JUN 2005

=> fil reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.21 0.21

this app
0 hits BEILSTEIN
0 hits CAPLUS

FILE 'REGISTRY' ENTERED AT 11:20:44 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3
DICTIONARY FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

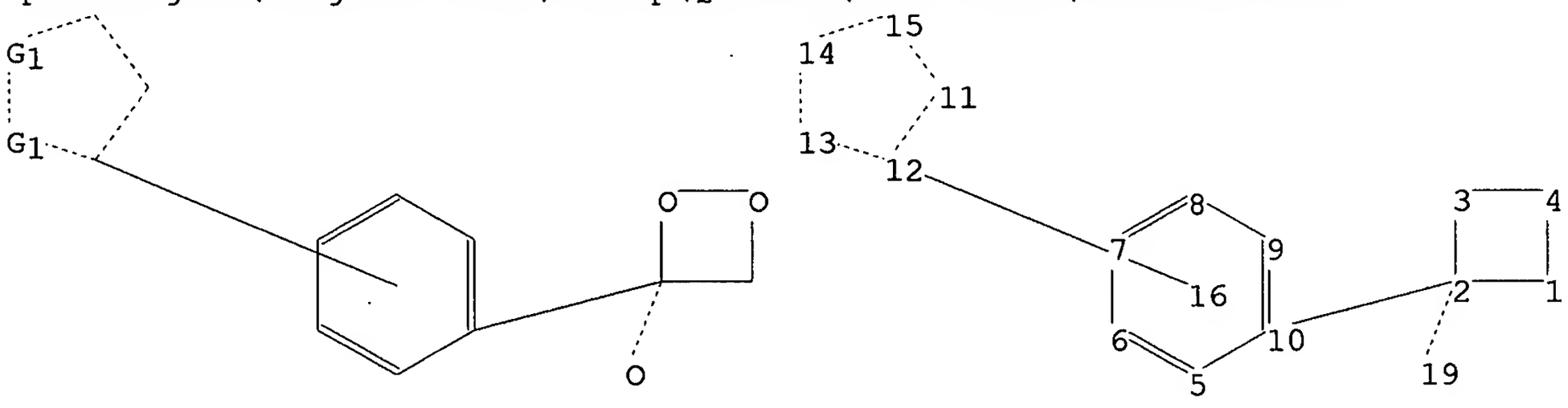
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\New Folder\10091447a.str



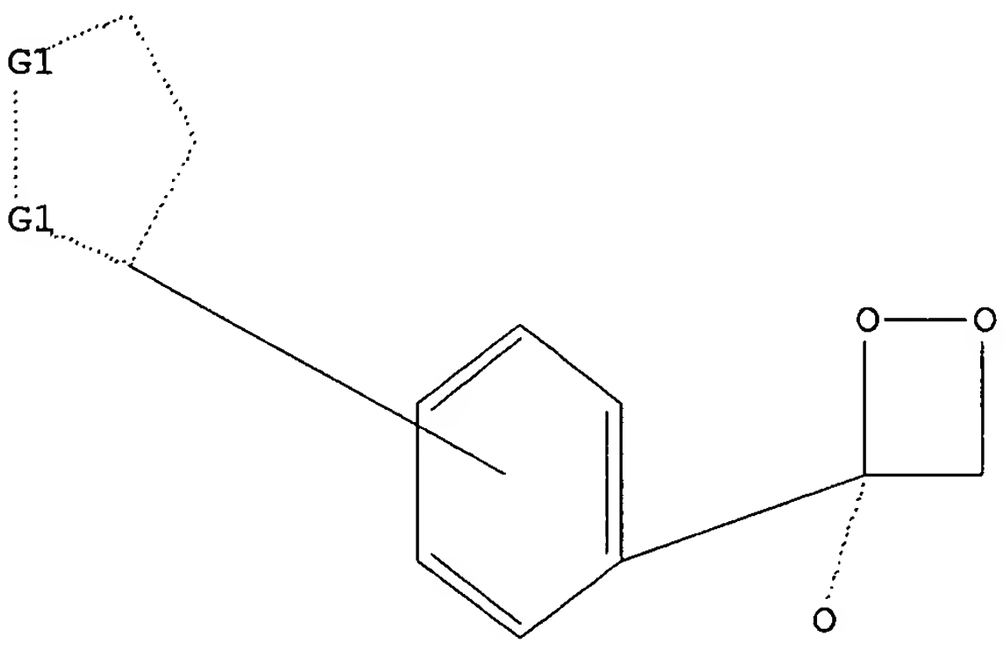
chain nodes :
19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
2-10 2-19
ring bonds :
1-2 1-4 2-3 3-4 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-15 12-13 13-14
14-15
exact/norm bonds :
1-2 1-4 2-3 2-10 2-19 3-4 11-12 11-15 12-13 13-14 14-15
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s L1
SAMPLE SEARCH INITIATED 11:21:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 8 TO 329
PROJECTED ANSWERS: 0 TO 0

```
L2             0 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 11:21:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     66 TO ITERATE

100.0% PROCESSED      66 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L3             0 SEA SSS FUL L1

=> fil beilstein
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.33     161.54

FILE 'BEILSTEIN' ENTERED AT 11:21:25 ON 03 JUN 2005
COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON APRIL 21, 2005

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS  9,218,366 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.

=> s L1 full
FULL SEARCH INITIATED 11:21:32 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED -      3 TO ITERATE

100.0% PROCESSED       3 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.05

L4             0 SEA SSS FUL L1
```

=> fil caold
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.06 | 161.60

FILE 'CAOLD' ENTERED AT 11:21:59 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s L1 full
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 11:22:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L1

L6 0 L5

=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.43 | 323.79

FILE 'REGISTRY' ENTERED AT 11:22:10 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3
DICTIONARY FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
**********************************************************
*                                                        *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                        *
**********************************************************
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.86	324.65

FILE 'REGISTRY' ENTERED AT 11:23:39 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3
DICTIONARY FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

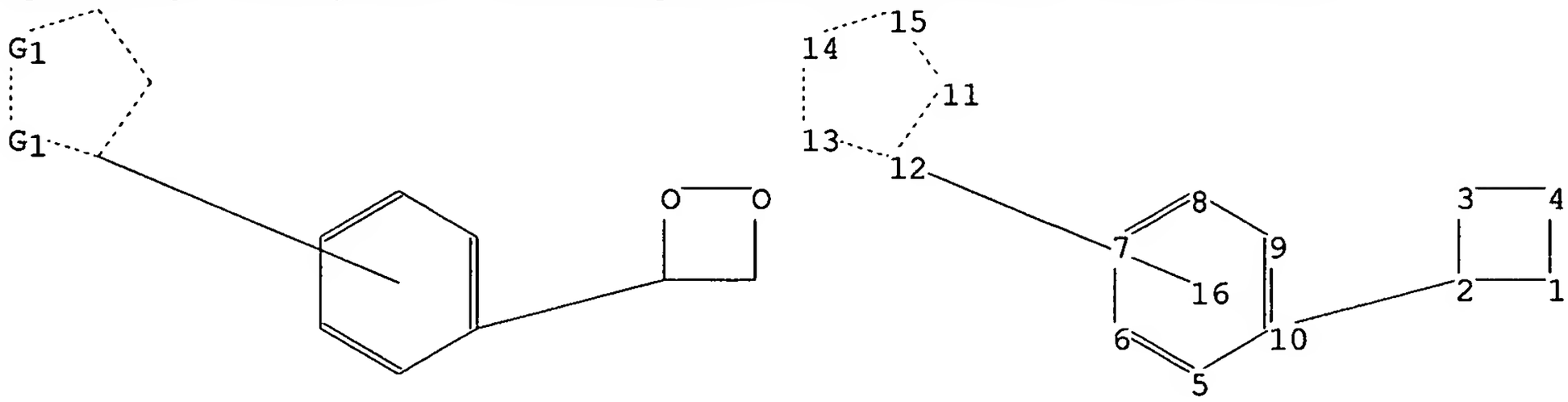
****
*   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now   *
* available and contains the CA role and document type information. *
*   *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\New Folder\10091447b.str



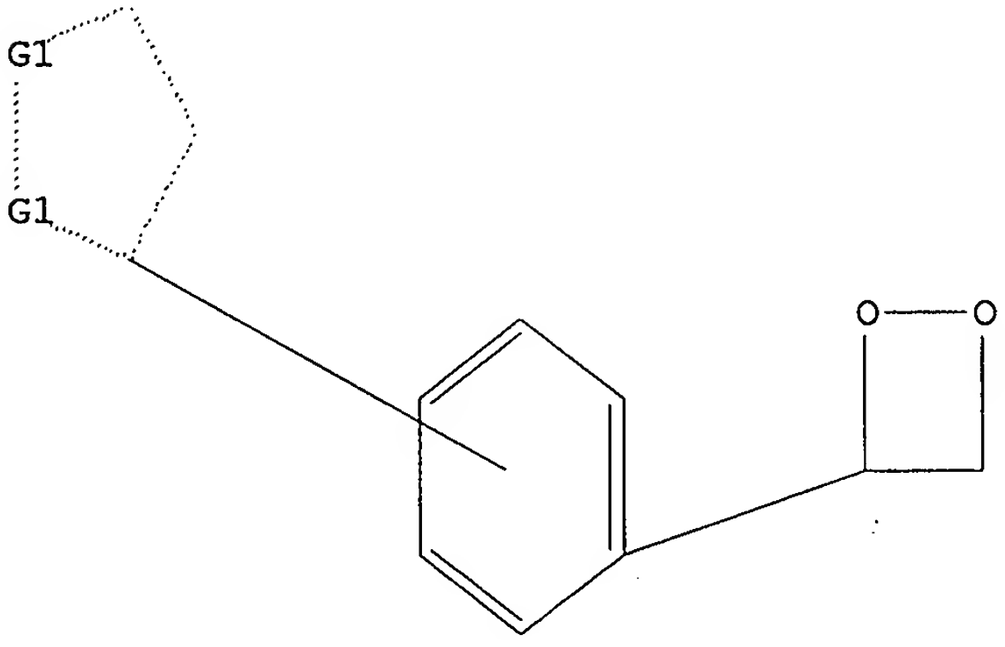
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
2-10
ring bonds :
1-2 1-4 2-3 3-4 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-15 12-13 13-14
14-15
exact/norm bonds :
1-2 1-4 2-3 2-10 3-4 11-12 11-15 12-13 13-14 14-15
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

```
=> s L7
SAMPLE SEARCH INITIATED 11:24:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     36 TO ITERATE

100.0% PROCESSED      36 ITERATIONS                                  1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          360 TO     1080
PROJECTED ANSWERS:               1 TO       80

L8             1 SEA SSS SAM L7

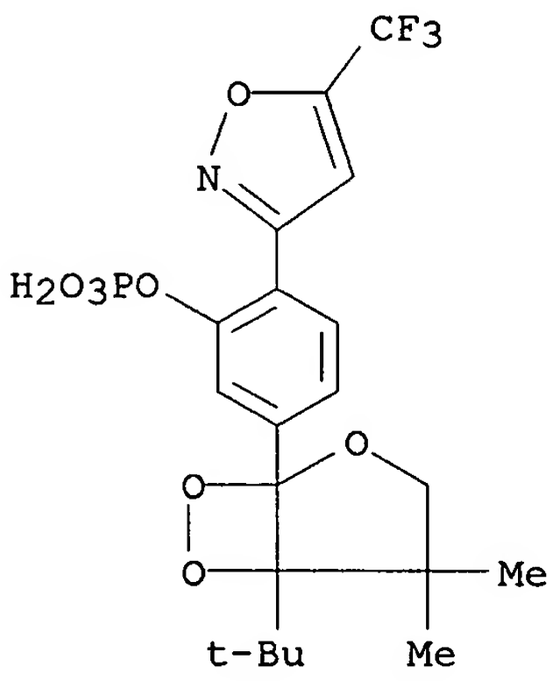
=> s L7 full
FULL SEARCH INITIATED 11:24:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    680 TO ITERATE

100.0% PROCESSED     680 ITERATIONS                                 6 ANSWERS
SEARCH TIME: 00.00.01

L9             6 SEA SSS FUL L7

=> d L9

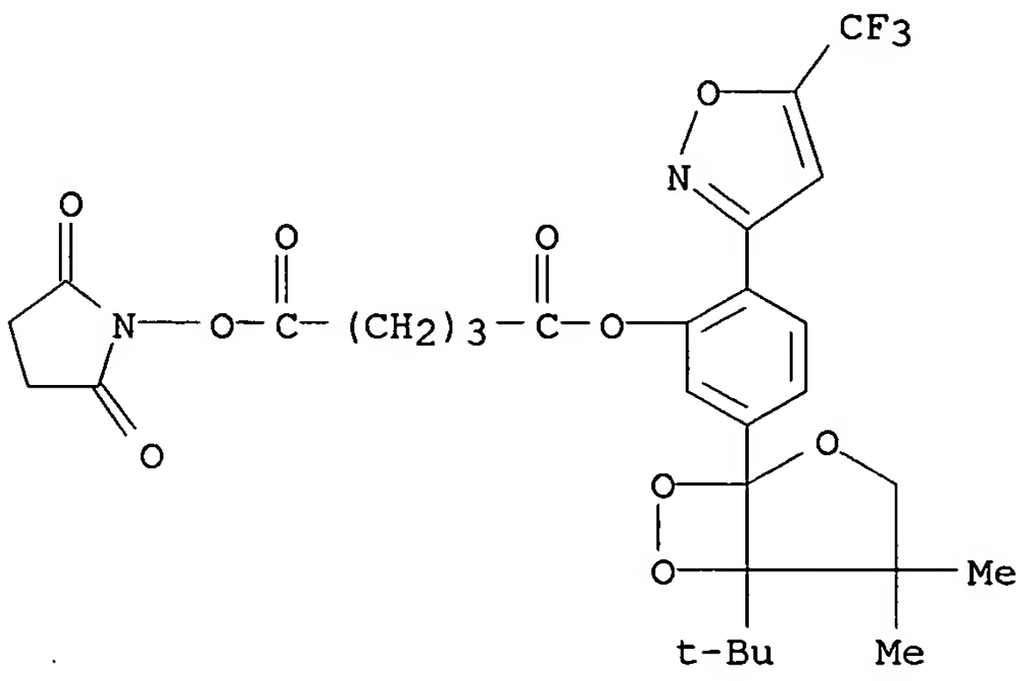
L9   ANSWER 1 OF 6  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   746599-91-7  REGISTRY
ED   Entered STN:  17 Sep 2004
CN   Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-
     trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]-,
     dihydrogen phosphate (ester) (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C20 H23 F3 N O8 P
CI   COM
SR   CA
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

=> d L9 2-6
```

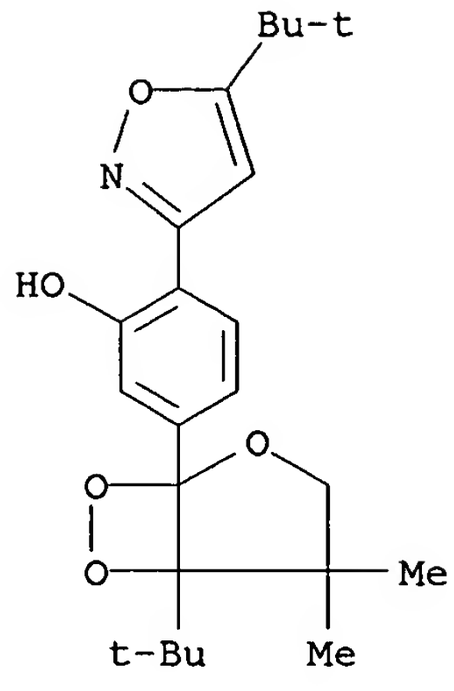
L9 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 594860-03-4 REGISTRY
ED Entered STN: 29 Sep 2003
CN Pentanoic acid, 5-[(2,5-dioxo-1-pyrrolidinyl)oxy]-5-oxo-,
    5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-
    2-[5-(trifluoromethyl)-3-isoxazolyl]phenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H31 F3 N2 O10
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

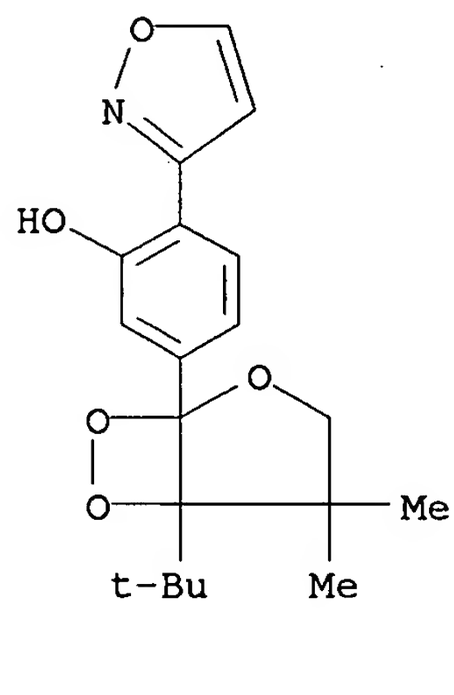
L9 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 502423-50-9 REGISTRY
ED Entered STN: 09 Apr 2003
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-
    trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(1,1-dimethylethyl)-3-isoxazolyl]-
    (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H31 N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 502423-49-6 REGISTRY
ED Entered STN: 09 Apr 2003
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-(3-isoxazolyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H23 N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT

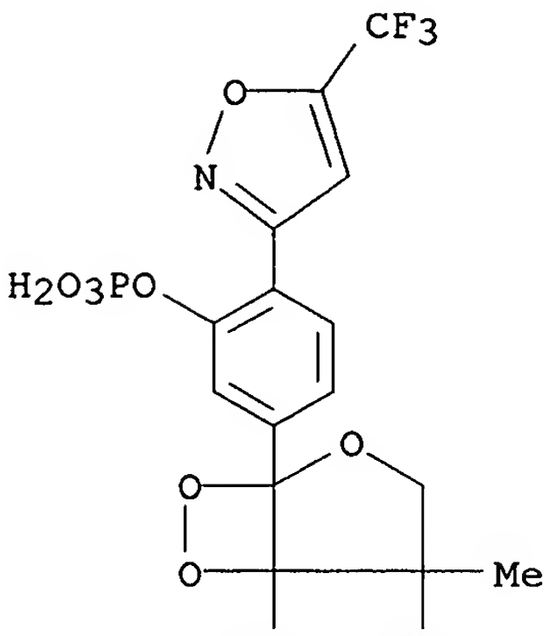


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 457898-62-3 REGISTRY
ED Entered STN: 02 Oct 2002
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)
MF C20 H23 F3 N O8 P . 2 Na

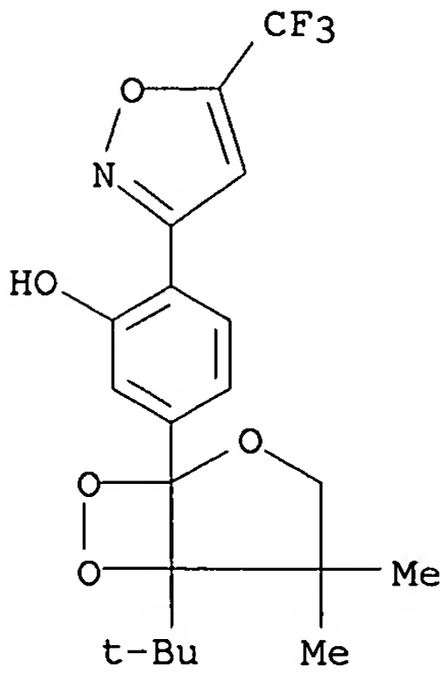
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
CRN (746599-91-7)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN 457898-58-7 REGISTRY
ED Entered STN: 02 Oct 2002
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H22 F3 N O5
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.80	497.45

FILE 'CAPLUS' ENTERED AT 11:25:05 ON 03 JUN 2005

FILE COVERS 1907 - 3 Jun 2005 VOL 142 ISS 24
FILE LAST UPDATED: 2 Jun 2005 (20050602/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L9
L10 3 L9

=> d ibib abs hitstr 1-3

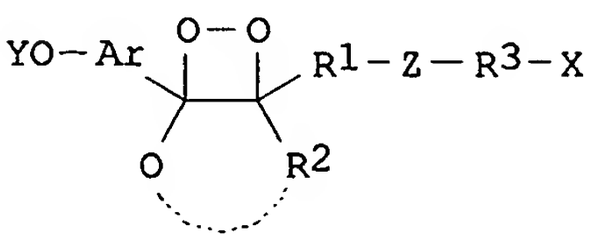
L10 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:717202 CAPLUS
DOCUMENT NUMBER: 139:230758
TITLE: 1,2-Dioxetane derivatives and chemiluminescent reagents employing them
INVENTOR(S): Matsumoto, Masakatsu; Watanabe, Nobuko; Yamada, Masashi
PATENT ASSIGNEE(S): Tosoh Corporation, Japan
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1342724	A1	20030910	EP 2003-4897	20030306
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004002300	A2	20040108	JP 2003-16454	20030124
US 2003207329	A1	20031106	US 2003-382853	20030307

US 6747160	B2	20040608			
US 2004176611	A1	20040909	US 2004-798338		20040312
US 6844453	B2	20050118			
PRIORITY APPLN. INFO.:			JP 2002-64040	A	20020308
			JP 2002-88380	A	20020327
			US 2003-382853	A3	20030307

OTHER SOURCE(S): MARPAT 139:230758

GI



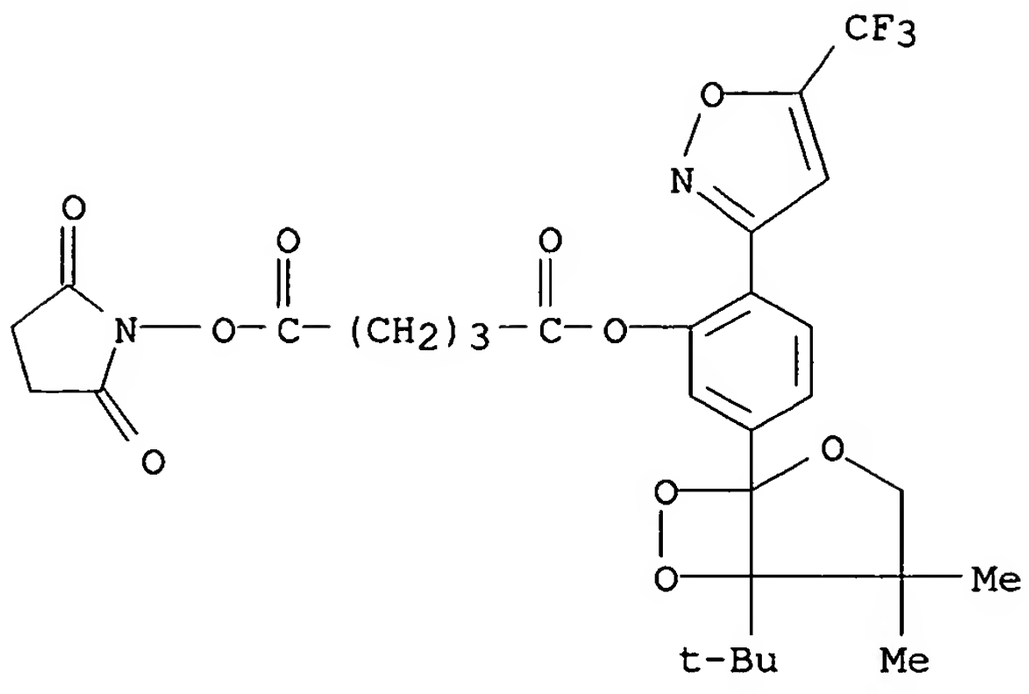
I

AB The patent relates to the preparation of A 1,2-dioxetane derivative of the formula (I): wherein Ar is an aryl group which may have an alkyl group, an aryl group, a halogen atom, an alkoxyl group, a carboxyl group, a formyl group, an alkyl ester, an aryl ester, an alkylketone, an arylketone or a hetero ring bonded thereto, X is a substituent capable of labeling an organic compound or a biol. mol., or an ester, Y is a hydrogen atom, an acyl group or a group of the formula -Si(R4R5R6) (wherein each of R4, R5 and R6 which are independent of one another, is an alkyl group or an aryl group), Z is an alkyl group, an aryl group, an oxygen atom, a sulfur atom, a carbonyl group, -(CO)-O-, -O-(CO)-, -NH-, -NH-CO-, -CO-NH-, -OSi(R7R8)- (wherein each of R7 and R8 which are independent of each other, is an alkyl group or aryl group) or a group of the formula -(R9R10) SiO- (wherein each of R9 and R10 which are independent of each other, is an alkyl group or an aryl group), each of R1 and R2 is an alkyl group or an aryl group, and R3 is a spacer. Thus, 1,2-dioxetane derivative 5-(5-tert-butyl-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl)-2-(5-trifluoromethylisooxazol-3-yl)phenylsuccinimidyl glutarate prepared in a multi-step synthesis was used with a TSH antibody (TSH antibody) to make a chemiluminescent substrate-labeled TSH antibody which is stable during anal. and can be handled easily.

IT **594860-03-4P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2-dioxetane derivs. and chemiluminescent reagents thereof for immunoassay)

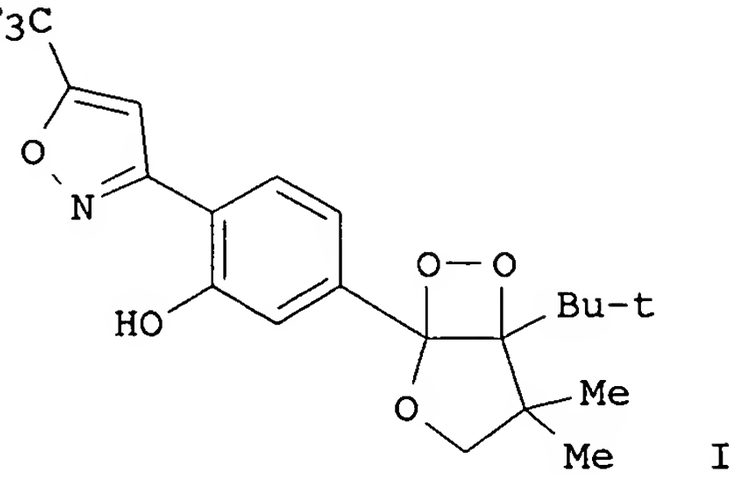
RN 594860-03-4 CAPLUS

CN Pentanoic acid, 5-[(2,5-dioxo-1-pyrrolidinyl)oxy]-5-oxo-, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]phenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:862396 CAPLUS
DOCUMENT NUMBER: 138:255129
TITLE: Synthesis of bicyclic dioxetanes bearing a 3-hydroxy-4-isoxazolylphenyl moiety: new CIEEL-active dioxetanes emitting light with remarkable high-efficiency in aqueous medium
AUTHOR(S): Matsumoto, Masakatsu; Sakuma, Toshimitsu; Watanabe, Nobuko
CORPORATE SOURCE: Department of Materials Science, Kanagawa University, Tsuchiya, Hiratsuka, Kanagawa, 259-1205, Japan
SOURCE: Tetrahedron Letters (2002), 43(49), 8955-8958
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:255129
GI



I

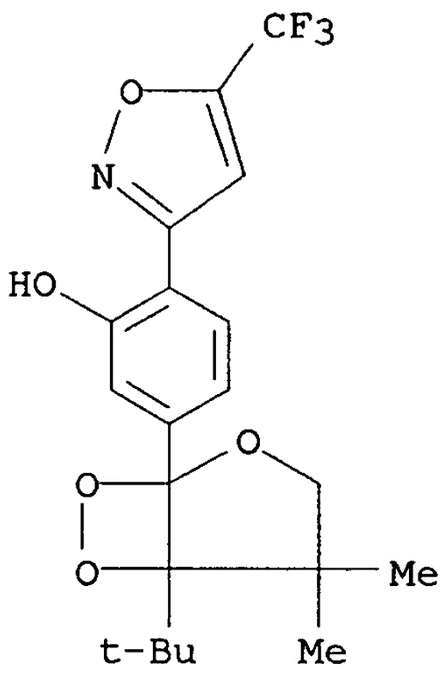
AB Bicyclic dioxetanes bearing a 3-hydroxy-4-isoxazolylphenyl moiety were synthesized. All these dioxetanes underwent base-induced CIEEL-decay to afford light with high efficiency in an NaOH/H2O system as well as in a TBAF (tetrabutylammonium fluoride)/acetonitrile system. Among them, a dioxetane bearing a 3-hydroxy-4-[5-(trifluoromethyl)isoxazol-3-yl]phenyl moiety (I) emitted light in the aqueous system with the highest efficiency which parallels that attained in an aprotic solvent system. Fluorescence study and the AM1 calcns. for I and the parent CIEEL-active dioxetanes

suggested that one important factor affecting chemiluminescence efficiency in an aqueous system should be the hydrogen-bonding at the carbonyl oxygen site of an oxyanion of hydroxyarenecarboxylate as the emitter produced by the CIEEL-decay.

IT **457898-58-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and AM1 calcns. of CIEEL-active bicyclic dioxetanes bearing a hydroxyisoxazolylphenyl moiety)

RN 457898-58-7 CAPLUS

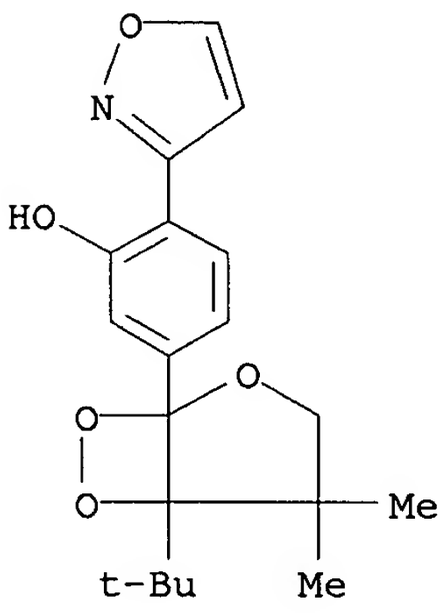
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)



IT **502423-49-6P 502423-50-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of CIEEL-active bicyclic dioxetanes bearing a hydroxyisoxazolylphenyl moiety)

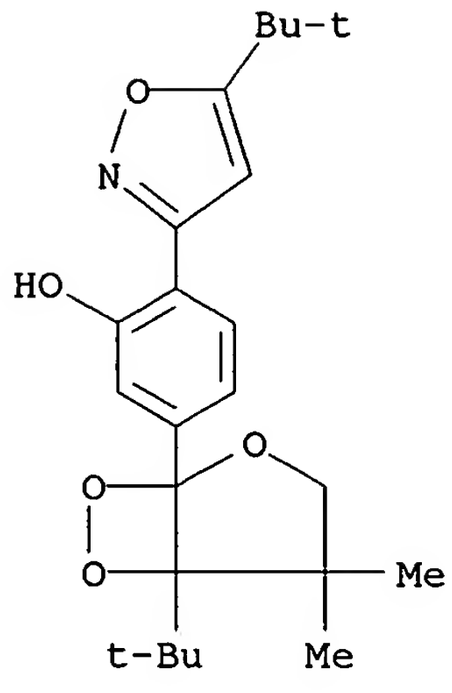
RN 502423-49-6 CAPLUS

CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-(3-isoxazolyl)- (9CI) (CA INDEX NAME)



RN 502423-50-9 CAPLUS

CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(1,1-dimethylethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)

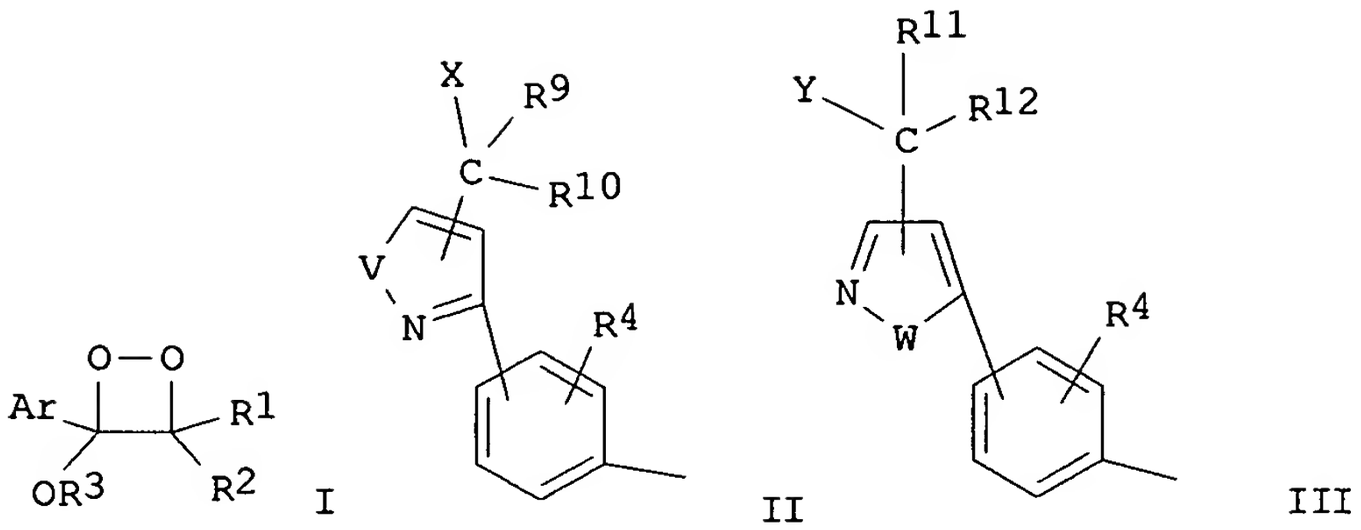


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:693160 CAPLUS
DOCUMENT NUMBER: 137:232640
TITLE: 1,2-dioxetane derivatives and their use as chemiluminescent reagents, luminescence methods and measuring methods
INVENTOR(S): Matsumoto, Masakatsu; Watanabe, Nobuko; Yamada, Masashi
PATENT ASSIGNEE(S): Tosoh Corporation, Japan
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1238976	A1	20020911	EP 2002-5225	20020307
EP 1238976	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002338576	A2	20021127	JP 2002-57606	20020304
US 2002132365	A1	20020919	US 2002-91447	20020307
PRIORITY APPLN. INFO.:			JP 2001-65347 A	20010308
OTHER SOURCE(S): MARPAT 137:232640				

GI

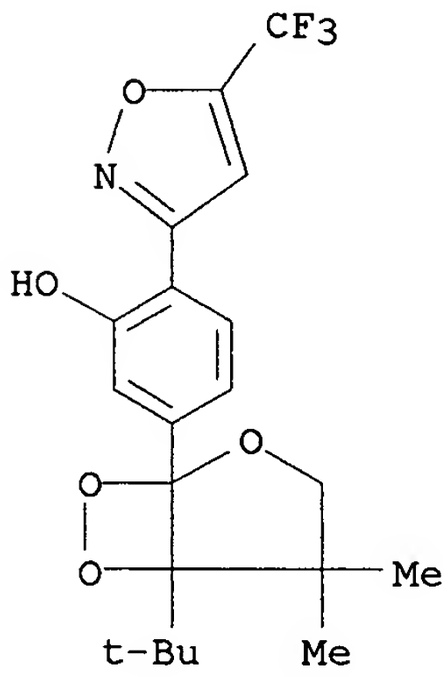


I II III

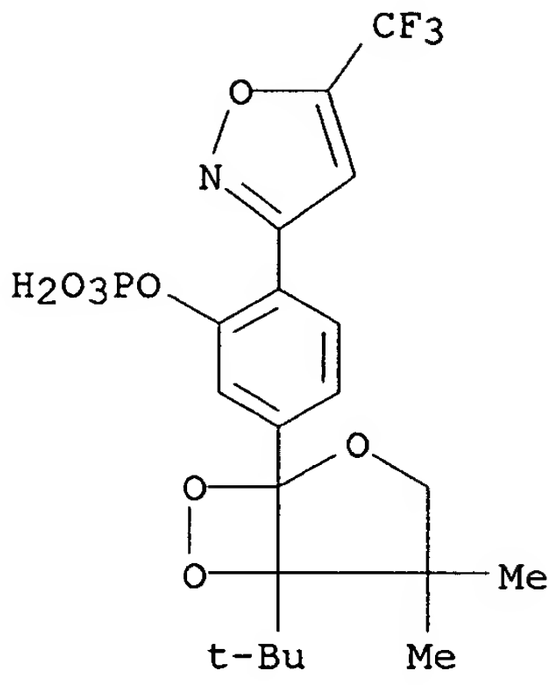
AB 1,2-Dioxetane derivs. are described by the general formula I (R1 and R2 = independently selected H, alkyl or aryl, or R1 and R2 may together form a cyclic or polycyclic organic ring group spiro-bonded to the dioxetane ring; R3 = alkyl or aryl, or R3 and R1 or R2 may together form a condensed ring containing the dioxetane ring and a heteroatom; Ar = II or III; R4 = OH, alkoxyl, aralkyloxy, -OSi(R5R6R7), phosphate, or -S(C:O)R8; R5, R6 and R7 = independently selected alkyl or aryl groups; R8 = alkyl or aryl; R9 and R10 = independently selected H, alkyl, aryl or halo; X = halo; V = O or S; R11 and R12 = independently selected H, alkyl, aryl or halo; Y = halo; and W = O or S). Chemiluminescent compns. incorporating the compds. are also described, as is their use in chemiluminescence anal. methods (e.g., immunoassays (no data)).

IT **457898-58-7P 457898-62-3P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); PREP (Preparation); USES (Uses)
(1,2-dioxetane derivs. and their use as chemiluminescent reagents and luminescence methods using them)

RN 457898-58-7 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)



RN 457898-62-3 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)



●2 Na

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil beilstein

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.72	513.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.19

FILE 'BEILSTEIN' ENTERED AT 11:26:08 ON 03 JUN 2005

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON APRIL 21, 2005

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS 9,218,366 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *

* FOR PRICE INFORMATION SEE HELP COST *
****

NEW
*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**
*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

=> s L7
SAMPLE SEARCH INITIATED 11:26:18 FILE 'BEILSTEIN'
SAMPLE SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 132 TO 668
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L7

=> fil casreact
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.06 513.23

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -2.19

FILE 'CASREACT' ENTERED AT 11:26:37 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 29 May 2005 VOL 142 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
* *
* CASREACT now has more than 9.2 million reactions *
* *
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L7
SAMPLE SEARCH INITIATED 11:26:41 FILE 'CASREACT'
SCREENING COMPLETE - 60 REACTIONS TO VERIFY FROM 5 DOCUMENTS

100.0% DONE 60 VERIFIED 0 HIT RXNS 0 DOCS

Connecting via Winsock to STN

10/09/447 6/3/05

Welcome to STN International! Enter x:x

LOGINID:[redacted]

Structure Search
3 hits CAPLUS
copending apps
Tetrahedron Letters
this app

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced
NEWS	16	APR 18	New CAS Information Use Policies available online
NEWS	17	APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAplus and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	18	APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAplus
NEWS	19	MAY 23	GBFULL enhanced with patent drawing images
NEWS	20	MAY 23	REGISTRY has been enhanced with source information from CHEMCATS
NEWS	21	MAY 26	STN User Update to be held June 6 and June 7 at the SLA 2005 Annual Conference

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:33:50 ON 03 JUN 2005

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:33:58 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3
DICTIONARY FILE UPDATES: 2 JUN 2005 HIGHEST RN 851586-61-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

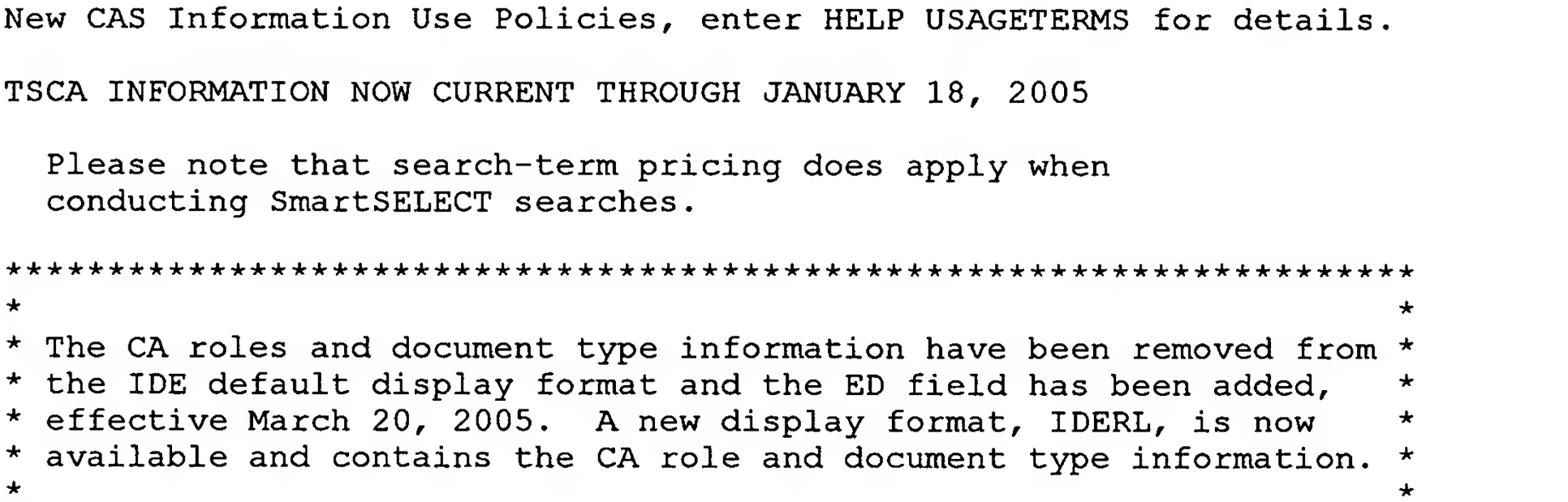
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\New Folder\10091447c.str



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ring nodes :
2  3  4  5  6  7  10  11  12  13  14  15  16  17  18  19  20
chain bonds :
3-15
ring bonds :
2-3  2-5  2-6  3-4  3-7  4-5  6-7  10-11  10-15  11-12  12-13  13-14  14-15  16-17
16-20  17-18  18-19  19-20
exact/norm bonds :
2-3  2-5  2-6  3-4  3-7  3-15  4-5  6-7  16-17  16-20  17-18  18-19  19-20
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15


G1:O,S,N

Match level :
2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  10:Atom  11:Atom  12:Atom  13:Atom
14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:CLASS
```

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L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1                STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s L1
SAMPLE SEARCH INITIATED 11:34:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED       6 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:             6 TO      266
PROJECTED ANSWERS:                1 TO       80

L2             1 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 11:34:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    109 TO ITERATE

100.0% PROCESSED     109 ITERATIONS                                 6 ANSWERS
SEARCH TIME: 00.00.01

L3             6 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   161.33     161.54

FILE 'CAPLUS' ENTERED AT 11:34:29 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 3 Jun 2005 VOL 142 ISS 24
FILE LAST UPDATED: 2 Jun 2005 (20050602/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s L3
L4              3 L3

=> d ibib abs hitstr
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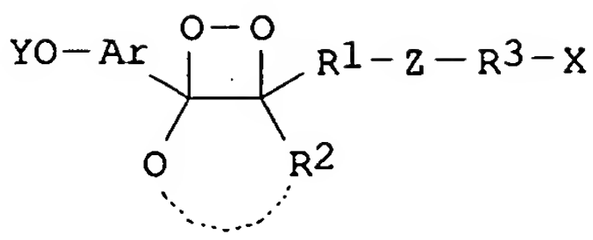
L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:717202 CAPLUS
DOCUMENT NUMBER: 139:230758
TITLE: 1,2-Dioxetane derivatives and chemiluminescent reagents employing them
INVENTOR(S): Matsumoto, Masakatsu; Watanabe, Nobuko; Yamada, Masashi
PATENT ASSIGNEE(S): Tosoh Corporation, Japan
SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

co-pending apps

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1342724	A1	20030910	EP 2003-4897	20030306
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004002300	A2	20040108	JP 2003-16454	20030124
US 2003207329	A1	20031106	US 2003-382853	20030307
US 6747160	B2	20040608		
US 2004176611	A1	20040909	US 2004-798338	20040312
US 6844453	B2	20050118		

PRIORITY APPLN. INFO.: JP 2002-64040 A 20020308
JP 2002-88380 A 20020327
US 2003-382853 A3 20030307

OTHER SOURCE(S): MARPAT 139:230758
GI



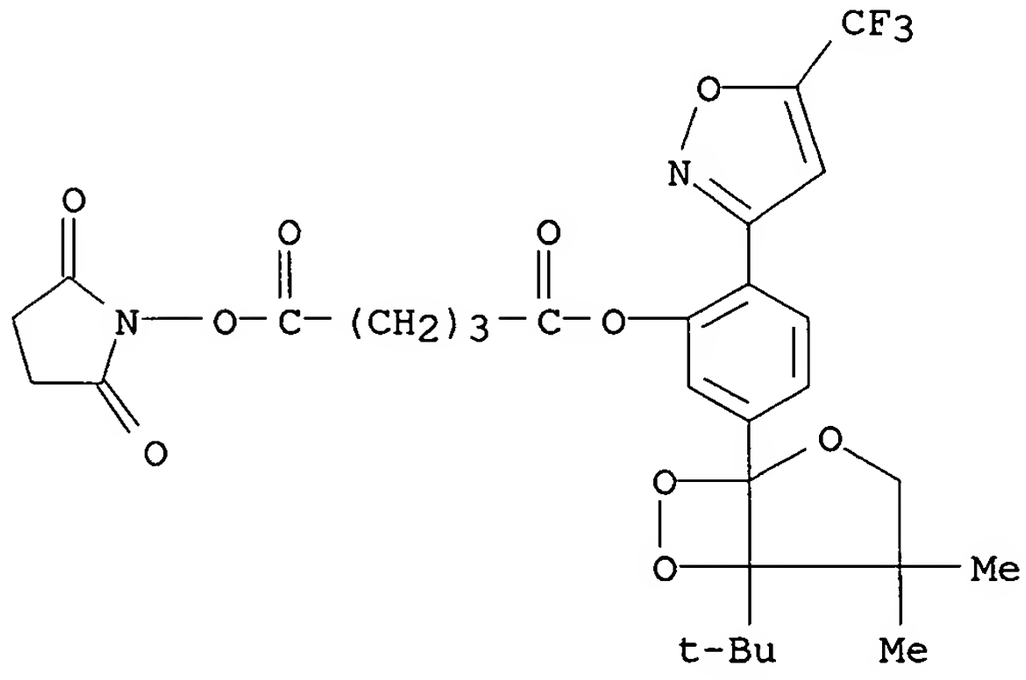
I

AB The patent relates to the preparation of A 1,2-dioxetane derivative of the formula (I): wherein Ar is an aryl group which may have an alkyl group, an aryl group, a halogen atom, an alkoxyl group, a carboxyl group, a formyl group, an alkyl ester, an aryl ester, an alkylketone, an arylketone or a hetero ring bonded thereto, X is a substituent capable of labeling an organic compound or a biol. mol., or an ester, Y is a hydrogen atom, an acyl group or a group of the formula -Si(R4R5R6) (wherein each of R4, R5 and R6 which are independent of one another, is an alkyl group or an aryl group), Z is an alkyl group, an aryl group, an oxygen atom, a sulfur atom, a carbonyl group, -(CO)-O-, -O-(CO)-, -NH-, -NH-CO-, -CO-NH-, -OSi(R7R8)- (wherein each of R7 and R8 which are independent of each other, is an alkyl group or aryl group) or a group of the formula -(R9R10) SiO- (wherein each of R9 and R10 which are independent of each other, is an alkyl group or an aryl group), each of R1 and R2 is an alkyl group or an aryl group, and R3 is a spacer. Thus, 1,2-dioxetane derivative 5-(5-tert-butyl-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl)-2-(5-trifluoromethylisooxazol-3-yl)phenylsuccinimidyl glutarate prepared in a multi-step synthesis was used with a TSH antibody (TSH antibody) to make a chemiluminescent substrate-labeled TSH antibody which is stable during anal. and can be handled easily.

IT **594860-03-4P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2-dioxetane derivs. and chemiluminescent reagents thereof for immunoassay)

RN 594860-03-4 CAPLUS

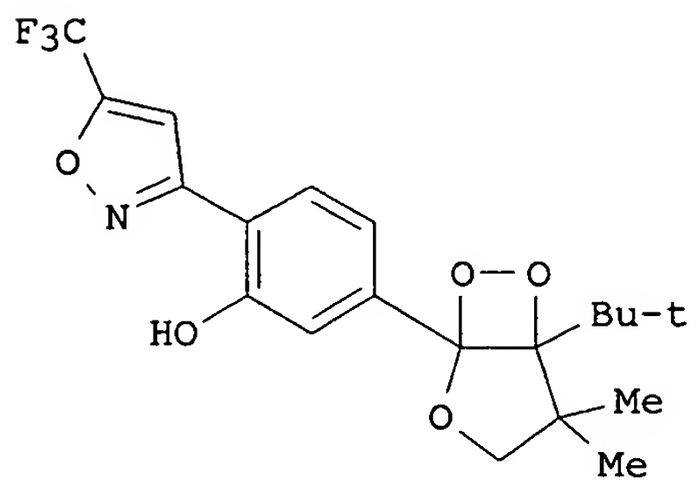
CN Pentanoic acid, 5-[(2,5-dioxo-1-pyrrolidinyl)oxy]-5-oxo-, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]phenyl ester (9CI) (CA INDEX NAME).



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2-3

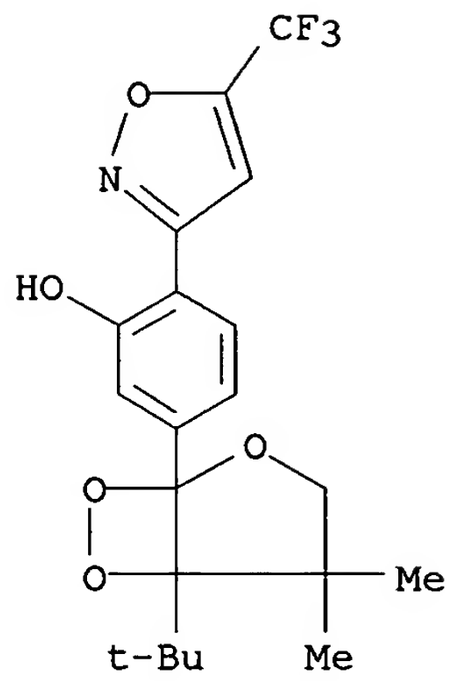
L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:862396 CAPLUS
DOCUMENT NUMBER: 138:255129
TITLE: Synthesis of bicyclic dioxetanes bearing a 3-hydroxy-4-isoxazolylphenyl moiety: new CIEEL-active dioxetanes emitting light with remarkable high-efficiency in aqueous medium
AUTHOR(S): Matsumoto, Masakatsu; Sakuma, Toshimitsu; Watanabe, Nobuko
CORPORATE SOURCE: Department of Materials Science, Kanagawa University, Tsuchiya, Hiratsuka, Kanagawa, 259-1205, Japan
SOURCE: Tetrahedron Letters (2002), 43(49), 8955-8958
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:255129
GI



I

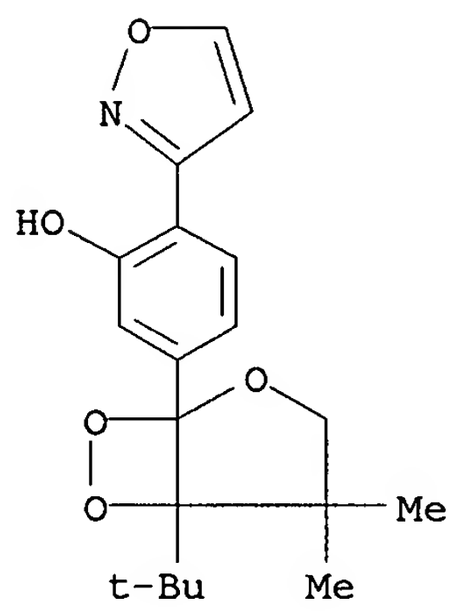
AB Bicyclic dioxetanes bearing a 3-hydroxy-4-isoxazolylphenyl moiety were synthesized. All these dioxetanes underwent base-induced CIEEL-decay to afford light with high efficiency in an NaOH/H2O system as well as in a TBAF (tetrabutylammonium fluoride)/acetonitrile system. Among them, a dioxetane bearing a 3-hydroxy-4-[5-(trifluoromethyl)isoxazol-3-yl]phenyl moiety (I) emitted light in the aqueous system with the highest efficiency which parallels that attained in an aprotic solvent system. Fluorescence study and the AM1 calcns. for I and the parent CIEEL-active dioxetanes suggested that one important factor affecting chemiluminescence efficiency in an aqueous system should be the hydrogen-bonding at the carbonyl oxygen site of an oxyanion of hydroxyarenecarboxylate as the emitter produced by the CIEEL-decay.

IT **457898-58-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and AM1 calcns. of CIEEL-active bicyclic dioxetanes bearing a hydroxyisoxazolylphenyl moiety)
RN 457898-58-7 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)

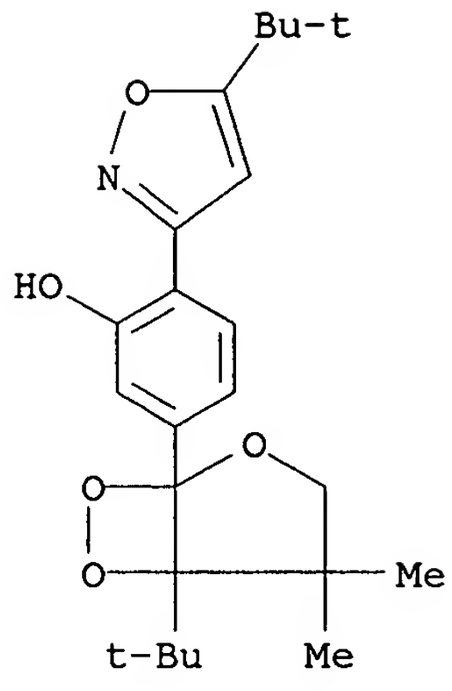


IT **502423-49-6P 502423-50-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of CIEEL-active bicyclic dioxetanes bearing a hydroxyisoxazolylphenyl moiety)

RN 502423-49-6 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-(3-isoxazolyl)- (9CI) (CA INDEX NAME)



RN 502423-50-9 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(1,1-dimethylethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:693160 CAPLUS
DOCUMENT NUMBER: 137:232640
TITLE: 1,2-dioxetane derivatives and their use as chemiluminescent reagents, luminescence methods and measuring methods
INVENTOR(S): Matsumoto, Masakatsu; Watanabe, Nobuko; Yamada, Masashi
PATENT ASSIGNEE(S): Tosoh Corporation, Japan
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1238976	A1	20020911	EP 2002-5225	20020307
EP 1238976	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002338576	A2	20021127	JP 2002-57606	20020304
US 2002132365	A1	20020919	US 2002-91447	20020307
PRIORITY APPLN. INFO.:			JP 2001-65347 A	20010308
OTHER SOURCE(S):			MARPAT 137:232640	

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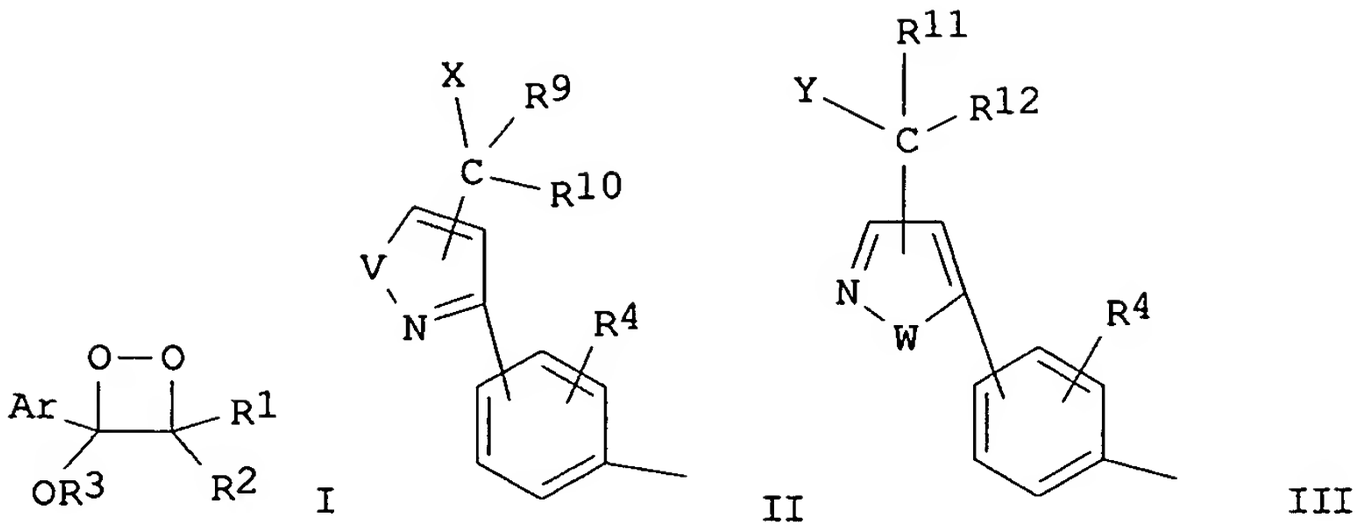
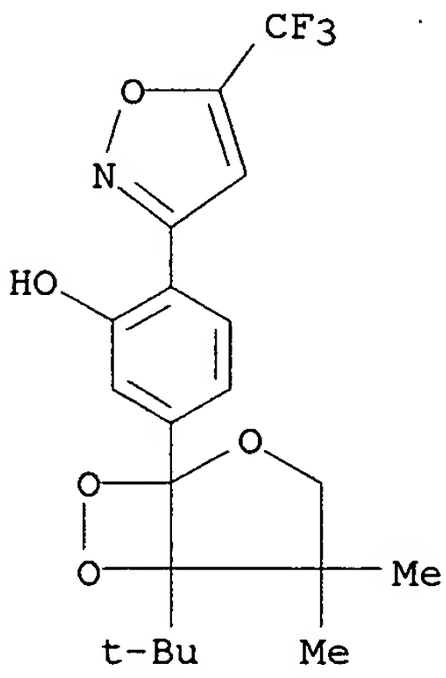


I II III

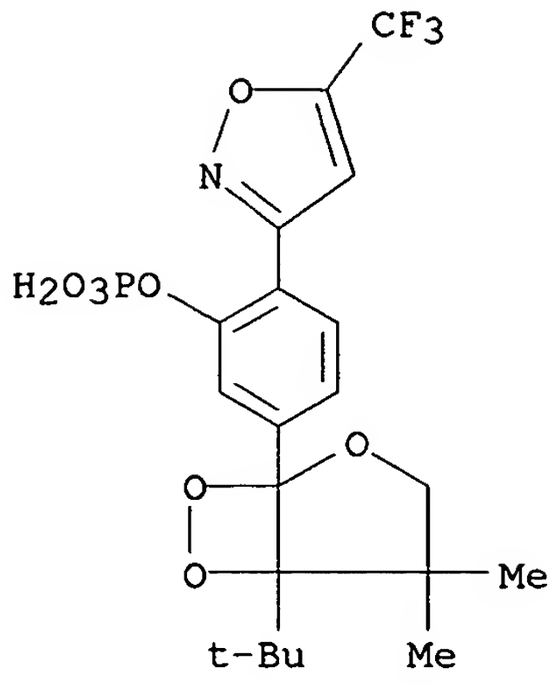
AB 1,2-Dioxetane derivs. are described by the general formula I (R1 and R2 = independently selected H, alkyl or aryl, or R1 and R2 may together form a cyclic or polycyclic organic ring group spiro-bonded to the dioxetane ring; R3 = alkyl or aryl, or R3 and R1 or R2 may together form a condensed ring containing the dioxetane ring and a heteroatom; Ar = II or III; R4 = OH, alkoxyl, aralkyloxy, -OSi(R5R6R7), phosphate, or -S(C:O)R8; R5, R6 and R7 = independently selected alkyl or aryl groups; R8 = alkyl or aryl; R9 and R10 = independently selected H, alkyl, aryl or halo; X = halo; V = O or S; R11 and R12 = independently selected H, alkyl, aryl or halo; Y = halo; and W = O or S). Chemiluminescent compns. incorporating the compds. are also described, as is their use in chemiluminescence anal. methods (e.g., immunoassays (no data)).

IT **457898-58-7P 457898-62-3P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); PREP (Preparation); USES (Uses)
(1,2-dioxetane derivs. and their use as chemiluminescent reagents and luminescence methods using them)

RN 457898-58-7 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]- (9CI) (CA INDEX NAME)



RN 457898-62-3 CAPLUS
CN Phenol, 5-[5-(1,1-dimethylethyl)-4,4-dimethyl-2,6,7-trioxabicyclo[3.2.0]hept-1-yl]-2-[5-(trifluoromethyl)-3-isoxazolyl]-, dihydrogen phosphate (ester), disodium salt (9CI) (CA INDEX NAME)



●2 Na

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	15.27	176.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.19

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6/3/05 10/091,477

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FILE 'HOME' ENTERED AT 16:40:50 ON 03 JUN 2005

text search dioxetanes & isoxazoles.

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 16:40:58 ON 03 JUN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 3 Jun 2005 VOL 142 ISS 24
FILE LAST UPDATED: 2 Jun 2005 (20050602/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 1,2-dioxetane?
       8285276 1
       8394030 2
          1492 DIOXETANE?
L1          815 1,2-DIOXETANE?
                  (1(W)2(W)DIOXETANE?)

=> s isooxazol? or 1,2-oxazol?
           237 ISOOXAZOL?
       8285276 1
       8394030 2
         38674 OXAZOL?
           214 1,2-OXAZOL?
                 (1(W)2(W)OXAZOL?)
L2          451 ISOOXAZOL? OR 1,2-OXAZOL?

=> s L1 and L2
L3            0 L1 AND L2

=> d L1 200 ibib kwic

L1   ANSWER 200 OF 815  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1997:588973  CAPLUS
DOCUMENT NUMBER:          127:255161
TITLE:                    Branched quantum chain processes in the reaction of
                          1,2-dioxetane with
                          Eu(fod)3 on a sorbent surface and in a solution
```

AUTHOR(S): Kazakov, V. P.; Voloshin, A. I.; Ostakhov, S. S.
CORPORATE SOURCE: Inst. Org. Khim., Ufim. Nauchn.Tsentra, RAN, Ufa, Russia
SOURCE: Doklady Akademii Nauk (1997), 354(1), 65-69
CODEN: DAKNEQ; ISSN: 0869-5652
PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

TI Branched quantum chain processes in the reaction of **1,2-dioxetane** with Eu(fod)3 on a sorbent surface and in a solution

AB Chemiluminescent reaction of adamantylideneadamantane-**1,2-dioxetane** with tris(heptafluorodimethyloctanedione)europium [Eu(fod)3] was studied in toluene solution and on a sorbent surface. The reaction proceeded via branched quantum chain involving Eu(fod)3 in excited 5D1 and 5D0 states.

IT Electronic energy transfer
Electronic energy transfer
Luminescence, chemiluminescence
(chain processes in chemiluminescent reaction of adamantylideneadamantane-**1,2-dioxetane** catalyzed with tris(heptafluorodimethyloctanedione)europium)

IT Reaction mechanism
(chain; chain processes in chemiluminescent reaction of adamantylideneadamantane-**1,2-dioxetane** catalyzed with tris(heptafluorodimethyloctanedione)europium)

IT 17631-68-4
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(chain processes in chemiluminescent reaction of adamantylideneadamantane-**1,2-dioxetane** catalyzed with tris(heptafluorodimethyloctanedione)europium)

IT 35544-39-9, Adamantylideneadamantane-**1,2-dioxetane**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(chain processes in chemiluminescent reaction of adamantylideneadamantane-**1,2-dioxetane** catalyzed with tris(heptafluorodimethyloctanedione)europium)

```
=> s dioxetan?
L4          1582 DIOXETAN?

=> s isozazole or isooxazole or 2(3a)oxazole
               7 ISOZAZOLE
               1 ISOZAZOLES
               8 ISOZAZOLE
                 (ISOZAZOLE OR ISOZAZOLES)
              65 ISOOXAZOLE
              17 ISOOXAZOLES
              79 ISOOXAZOLE
                 (ISOOXAZOLE OR ISOOXAZOLES)
         8394030 2
            6621 OXAZOLE
            2147 OXAZOLES
            7482 OXAZOLE
                 (OXAZOLE OR OXAZOLES)
            2171 2(3A)OXAZOLE
L5          2258 ISOZAZOLE OR ISOOXAZOLE OR 2(3A)OXAZOLE

=> s isoxazole or isooxazole or 2(3a)oxazole
            6458 ISOXAZOLE
            2258 ISOXAZOLES
```

```
          7196 ISOXAZOLE
                 (ISOXAZOLE OR ISOXAZOLES)
            65 ISOOXAZOLE
            17 ISOOXAZOLES
            79 ISOOXAZOLE
                 (ISOOXAZOLE OR ISOOXAZOLES)
       8394030 2
          6621 OXAZOLE
          2147 OXAZOLES
          7482 OXAZOLE
                 (OXAZOLE OR OXAZOLES)
          2171 2(3A)OXAZOLE
L6        9335 ISOXAZOLE OR ISOOXAZOLE OR 2(3A)OXAZOLE

=> s L4 and L6
L7           0 L4 AND L6

=> s isoxazol? or isooxazol? or 2(3a)oxazol?
         17808 ISOXAZOL?
           237 ISOOXAZOL?
       8394030 2
         38674 OXAZOL?
         19713 2(3A)OXAZOL?
L8       37038 ISOXAZOL? OR ISOOXAZOL? OR 2(3A)OXAZOL?

=> s L4 and L8
L9           10 L4 AND L8

=> d ibib abs 1-10

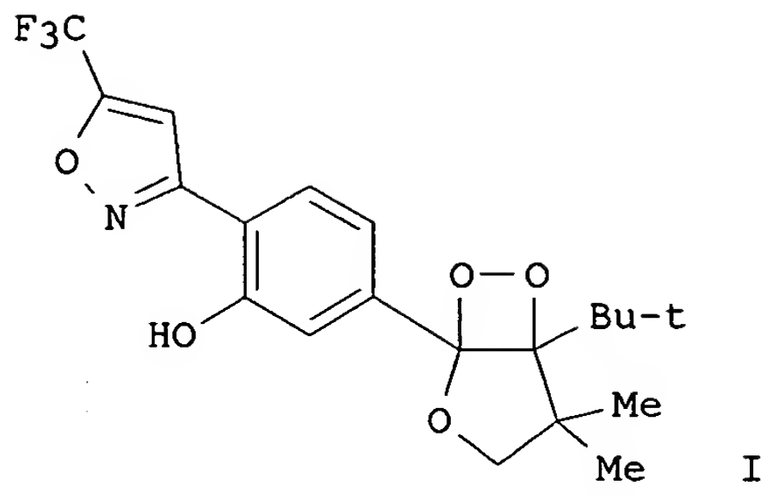
L9   ANSWER 1 OF 10  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2005:78081  CAPLUS
DOCUMENT NUMBER:          142:151541
TITLE:                    Sequential generation of multiple chemiluminescent
                          signals on solid supports
INVENTOR(S):              Voyta, John C.; Smith, Robert M.; Schroth, Gary P.;
                          Sparks, Alison L.; Edwards, Brooks N.; Gonzalez,
                          Carolyn
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 9 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     US 2005019778         A1    20050127    US 2003-620332           20030717
     WO 2005007874         A2    20050127    WO 2004-US23081          20040719
     WO 2005007874         A3    20050331
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
PRIORITY APPLN. INFO.:                    US 2003-620332      A  20030717
```

AB Chemiluminescent assays to determine the presence and/or amount of one or more labeled analytes in a sample are described wherein a solid support is contacted sequentially with first and second chemiluminescent substrates each of which are capable of being activated by an enzyme and the resulting chemiluminescent signals are detected. A plurality of probes are disposed on a surface layer of the solid support in a plurality of discrete areas. Some of the probes are bound to a conjugate of the first enzyme and some of the probes are bound to a conjugate of the second enzyme. The assay can be used to compare biol. samples (e.g., mRNA populations from different cells) on the same support surface. Alternatively, one of the chemiluminescent signals generated can be used as a control signal for normalizing the chemiluminescent assay data.

L9 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:922813 CAPLUS
DOCUMENT NUMBER: 140:110935
TITLE: Stereochemical Features of the Physical and Chemical Interactions of Singlet Oxygen with Enecarbamates
AUTHOR(S): Poon, Thomas; Turro, Nicholas J.; Chapman, Jessica; Lakshminarasimhan, P.; Lei, Xuegong; Jockusch, Steffen; Franz, Roberto; Washington, Ilyas; Adam, Waldemar; Bosio, Sara G.
CORPORATE SOURCE: Department of Chemistry and Department of Chemical Engineering, Columbia University, New York, NY, 10027, USA
SOURCE: Organic Letters (2003), 5(26), 4951-4953
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:110935
AB Oxazolidinone-substituted enecarbamates represent a mechanistically rich system for the study of stereoelectronic, steric, and conformational effects on stereoselectivity and mode selectivity in 1O2 [2 + 2] and ene reactions. Photooxygenation of these enecarbamates with 1O2 leads to diastereomerically pure **dioxetanes** that decompose to yield an oxazolidinone carbaldehyde and one of the two enantiomers of methyldesoxybenzoin in enantiomeric excess. Stereoselectivity originates at the allylic stereocenter, a result supported by quenching studies, computational anal., and deuterium solvent isotope effects.
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:862396 CAPLUS
DOCUMENT NUMBER: 138:255129
TITLE: Synthesis of bicyclic **dioxetanes** bearing a 3-hydroxy-4-**isoxazolylphenyl** moiety: new CIEEL-active **dioxetanes** emitting light with remarkable high-efficiency in aqueous medium
AUTHOR(S): Matsumoto, Masakatsu; Sakuma, Toshimitsu; Watanabe, Nobuko
CORPORATE SOURCE: Department of Materials Science, Kanagawa University, Tsuchiya, Hiratsuka, Kanagawa, 259-1205, Japan
SOURCE: Tetrahedron Letters (2002), 43(49), 8955-8958
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:255129
GI



I

AB Bicyclic **dioxetanes** bearing a 3-hydroxy-4-**isoxazolylphenyl** moiety were synthesized. All these **dioxetanes** underwent base-induced CIEEL-decay to afford light with high efficiency in an NaOH/H2O system as well as in a TBAF (tetrabutylammonium fluoride)/acetonitrile system. Among them, a **dioxetane** bearing a 3-hydroxy-4-[5-(trifluoromethyl) **isoxazol**-3-yl]phenyl moiety (I) emitted light in the aqueous system with the highest efficiency which parallels that attained in an aprotic solvent system. Fluorescence study and the AM1 calcns. for I and the parent CIEEL-active **dioxetanes** suggested that one important factor affecting chemiluminescence efficiency in an aqueous system should be the hydrogen-bonding at the carbonyl oxygen site of an oxyanion of hydroxyarenecarboxylate as the emitter produced by the CIEEL-decay.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:511737 CAPLUS
DOCUMENT NUMBER: 137:216900
TITLE: Highly Diastereoselective **Dioxetane** Formation in the Photooxygenation of Enecarbamates with an Oxazolidinone Chiral Auxiliary: Steric Control in the [2 + 2] Cycloaddition of Singlet Oxygen through Conformational Alignment
AUTHOR(S): Adam, Waldemar; Bosio, Sara G.; Turro, Nicholas J.
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany
SOURCE: Journal of the American Chemical Society (2002), 124(30), 8814-8815
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:216900

AB The photooxygenation of oxazolidinone-substituted enecarbamates leads to diastereomerically pure **dioxetanes**. The high diastereoselectivity is rationalized in terms of effective π-facial control achieved by shielding one side of the double bond with the chiral auxiliary. The absolute configuration of the **dioxetanes** is assigned by derivatization to diols.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

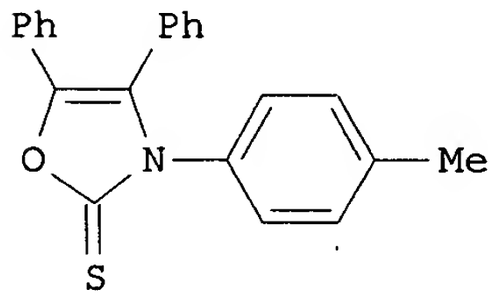
L9 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:389792 CAPLUS
DOCUMENT NUMBER: 133:150167
TITLE: Rearrangement Pathways of Arylperoxy Radicals. 2. Five-Membered Heterocycles
AUTHOR(S): Fadden, Michael J.; Hadad, Christopher M.

CORPORATE SOURCE: Department of Chemistry, The Ohio State University, Columbus, OH, 43210, USA
SOURCE: Journal of Physical Chemistry A (2000), 104(26), 6324-6331
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The potential energy surfaces for the reaction of furanyl and oxazolyl radicals with O2 have been examined using the B3LYP method. The initial production of the arylperoxy radical followed by either simple decomposition or rearrangement to yield several intermediates (aryloxy, dioxiranylaryl, or **dioxetanylaryl** radicals) has been explored. Transition state structures for most of the steps are presented as well as relative free energies over a range of temps. from 298 to 2000 K. The energetics of the analogous intermediates for the reaction of O2 and other five-membered heterocyclic radicals derived from pyrrole and thiophene are also provided. The loss of an O atom is generally the most accessible and energetically favored pathway of decomposition at all temps. Dioxiranyl formation is favored over O2 loss at temps. ≤500 K and favored in the same temperature range over O atom loss in several cases. **Dioxetanyl** formation incurs the greatest barrier to formation, and direct routes are not available in every mol. surveyed. However, in some cases the **dioxetane** radicals transform rapidly into very stable species.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:109624 CAPLUS
DOCUMENT NUMBER: 132:308271
TITLE: Photooxidative cleavage of **oxazoline**-**2**-thione in protic and aprotic solvents
AUTHOR(S): Singh, Indra Sen
CORPORATE SOURCE: Chemical Engineering Department, School of Technology, Copperbelt University, Kitwe, Zambia
SOURCE: Bulletin of the Chemical Society of Ethiopia (1999), 13(2), 127-133
CODEN: BCETE6; ISSN: 1011-3924
PUBLISHER: Chemical Society of Ethiopia
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:308271
GI



I

AB The photolysis of 4,5-diphenyl-3-(4-methylphenyl)-4-**oxazoline**-**2**-thione (I) in benzene or cyclohexane in the presence of singlet oxygen, using a Pyrex filtered 450 W Hanovia lamp, afforded benzil, N-(4-methylphenyl)benzamide, and N,N-dibenzoyl-4-methylaniline. When the same reaction was performed in protic solvents, the formation of benzil, N-(4-methylphenyl)benzamide, N,N-dibenzoyl-4-methylaniline, and benzoic acid was observed The products were characterized by spectral data and

comparison (undepressed m.ps. and identical IR spectra) with authentic samples. Oxazolines are a widely used class of compds., and therefore it would be relevant to study the effect of UV light on such compds. under different conditions. The present study derives an interesting route for the photooxidative fragmentation of the 4-**oxazoline-2**-thione ring system. It involves a **dioxetane** derivative, which, after cleavage, gives two radicals, which finally give the above products. The yield of N-(4-methylphenyl)benzamide is increased by protic solvents, which gives strong support to the proposed mechanism.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:546523 CAPLUS
DOCUMENT NUMBER: 125:269847
TITLE: Enhancement of chemiluminescent assays
INVENTOR(S): Bronstein, Irena Y.; Edwards, Brooks; Voyta, John C.
PATENT ASSIGNEE(S): Tropix, Inc., USA
SOURCE: U.S., 21 pp., Cont.-in-part of U.S. Ser. No. 959,531.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5547836	A	19960820	US 1993-31471	19930315
US 5112960	A	19920512	US 1990-574786	19900830
JP 04124185	A2	19920424	JP 1990-239764	19900910
JP 11021285	A2	19990126	JP 1996-86324	19910830
US 5330900	A	19940719	US 1991-806928	19911212
ES 2131529	T3	19990801	ES 1992-915721	19920305
US 5639907	A	19970617	US 1992-959531	19921013
CA 2157917	AA	19940929	CA 1994-2157917	19940315
WO 9421821	A1	19940929	WO 1994-US2549	19940315
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, TT, UA, UZ, VN				
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AU 9464449	A1	19941011	AU 1994-64449	19940315
EP 689611	A1	19960103	EP 1994-912204	19940315
EP 689611	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08507694	T2	19960820	JP 1994-521100	19940315
JP 3632856	B2	20050323		
EP 1120652	A1	20010801	EP 2001-102819	19940315
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AT 212722	E	20020215	AT 1994-912204	19940315
US 5543295	A	19960806	US 1994-233085	19940425
US 5679802	A	19971021	US 1995-433996	19950504
US 5654154	A	19970805	US 1996-588260	19960118
US 5831102	A	19981103	US 1996-598353	19960208
US 5994073	A	19991130	US 1997-850009	19970501
US 5856522	A	19990105	US 1997-882330	19970625
PRIORITY APPLN. INFO.:			US 1990-574786	A3 19900830
			US 1991-806928	A2 19911212
			US 1992-959531	A2 19921013
			US 1989-367772	B3 19850515
			US 1986-889823	A1 19860724
			US 1987-140197	B2 19871231
			US 1990-559152	A2 19900725

JP 1991-518245	A3	19910830
EP 1992-915721	A	19920305
US 1993-31471	A	19930315
EP 1994-912204	A3	19940315
WO 1994-US2549	W	19940315
US 1994-233085	A1	19940425
US 1995-433996	A1	19950504
US 1996-588260	A1	19960118

OTHER SOURCE(S): MARPAT 125:269847

AB Chemiluminescent bioassays for the detection or quantitation of an analyte in a sample use 1,2-**dioxetanes** as substrates for the enzyme of an enzyme complex that binds to the analyte. The chemiluminescence obtained from the decomposition of the **dioxetane** triggered by the enzyme through the formation of the corresponding 1,2-**dioxetane** oxyanion of the enzyme complex is enhanced by the addition of TBQ [poly(vinylbenzyltributylammonium chloride)] as an enhancement agent. Other polymeric quaternary onium salts can be used as enhancement agents in conjunction with enhancement additives which improve the ability of the enhancement agent to form hydrophobic regions in the aqueous sample, in which regions the 1,2-**dioxetane** oxyanion and its chemiluminescent decomposition products can be sequestered. A kit for performing such assays is also provided.

L9 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:169405 CAPLUS
DOCUMENT NUMBER: 122:260545
TITLE: Additives for enhancing chemiluminescent assays using 1,2-**dioxetanes** as substrates
INVENTOR(S): Bronstein, Irena Y.; Edwards, Brooks; Voyta, John C.
PATENT ASSIGNEE(S): Tropix, Inc., USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9421821	A1	19940929	WO 1994-US2549	19940315
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, TT, UA, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ES 2131529	T3	19990801	ES 1992-915721	19920305
US 5547836	A	19960820	US 1993-31471	19930315
CA 2157917	AA	19940929	CA 1994-2157917	19940315
AU 9464449	A1	19941011	AU 1994-64449	19940315
EP 689611	A1	19960103	EP 1994-912204	19940315
EP 689611	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08507694	T2	19960820	JP 1994-521100	19940315
JP 3632856	B2	20050323		
AT 212722	E	20020215	AT 1994-912204	19940315
US 5856522	A	19990105	US 1997-882330	19970625

PRIORITY APPLN. INFO.:

US 1993-31471	A	19930315
US 1990-574786	A3	19900830
US 1991-806928	A2	19911212
EP 1992-915721	A	19920305
US 1992-959531	A2	19921013
WO 1994-US2549	W	19940315
US 1995-433996	A1	19950504

OTHER SOURCE(S): MARPAT 122:260545

AB Disclosed is additives for enhancing chemiluminescent bioassays for the presence or concentration of an analyte in a sample use 1,2-**dioxetanes** as substrates for the enzyme of an enzyme complex that bind to the analyte. The additives include surfactant (e.g. Tween 20), solvent (e.g. isopropanol, polyvinyl alc.), and water-soluble polymers (e.g. polymeric quaternary onium salts). The chemiluminescence obtained from the decomposition of the **dioxetane** triggered by the enzyme through the formation of the corresponding 1,2-**dioxetane** oxyanion of the enzyme complex is enhanced by the addition of poly(vinylbenzyltributylammonium chloride) as an enhancement agent. Other polymeric quaternary onium salts can be used as enhancement agents in conjunction with enhancement additives which improve the ability of the enhancement agent to form hydrophobic regions in the aqueous sample, in which regions the 1,2-**dioxetane** oxyanion and its chemiluminescent decomposition products can be sequestered. A kit for performing such assays is also provided.

L9 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:173921 CAPLUS

DOCUMENT NUMBER: 94:173921

TITLE: Photochemical transformations of 4,5-diaryl-4-**oxazolin**-2-one protecting groups

AUTHOR(S): Guziec, Frank S., Jr.; Tewes, Edwin T.

CORPORATE SOURCE: Dep. Chem., Tufts Univ., Medford, MA, 02155, USA

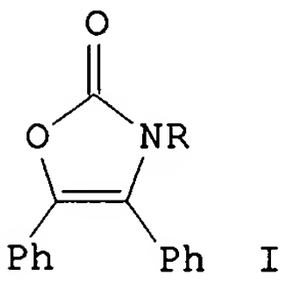
SOURCE: Journal of Heterocyclic Chemistry (1980), 17(8), 1807-8
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:173921

GI



I

AB UV irradiation in air of oxazolinones I (R = PhCH2CH2 or CH2CO2H) in MeOH leads to photooxidn. of the protecting group, affording the PhCONHR and PhCO2Me. Reduction of the intermediate **dioxetane** leads to complete removal of the protecting group. A mechanism for this photolysis is proposed and evidence in support of this mechanism is reported.

L9 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:446476 CAPLUS

DOCUMENT NUMBER: 85:46476

TITLE: Photochemistry of heterocyclic compounds. VI. The photochemical reaction of 3,4,5-triphenyl-4-**oxazolin**-2-one

AUTHOR(S): Tsuge, Otohiko; Oe, Koji; Ueyama, Yasuo

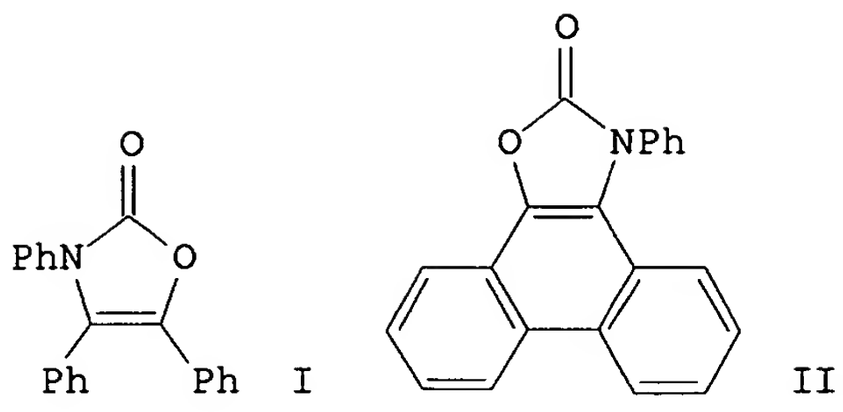
CORPORATE SOURCE: Res. Inst. Ind. Sci., Kyushu Univ., Fukuoka, Japan

SOURCE: Chemistry Letters (1976), (5), 425-8
CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

II

AB Irradiation of 3,4,5-triphenyl-4-**oxazolin**-**2**-one (I) in benzene under N with or without iodine gave PhCONHPh and phenanthroxazolinone II whereas in the presence of O I was photochem. converted to PhCONHPh, PhCO2H, and benzamidobenzophenones, presumably via an initial attack of singlet O to I followed by ring cleavage of the resulting **dioxetane** to give PhNBz2, which on irradiation gave the final products.

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E2            2     BRONSTEIN HOWARD D/AU
E3           23 --> BRONSTEIN I/AU
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E9           61     BRONSTEIN IRENA/AU
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L11          59 L10 AND DIOXETAN?

=> s L11 and ?oxazol?
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L12           5 L11 AND ?OXAZOL?

=> d L12 1-5 ibib abs

L12  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1996:546523  CAPLUS
DOCUMENT NUMBER:          125:269847
TITLE:                    Enhancement of chemiluminescent assays
INVENTOR(S):              Bronstein, Irena Y.; Edwards, Brooks; Voyta,
                          John C.
PATENT ASSIGNEE(S):       Tropix, Inc., USA
SOURCE:                   U.S., 21 pp., Cont.-in-part of U.S. Ser. No. 959,531.
                          CODEN: USXXAM
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
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FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5547836	A	19960820	US 1993-31471	19930315
US 5112960	A	19920512	US 1990-574786	19900830
JP 04124185	A2	19920424	JP 1990-239764	19900910
JP 11021285	A2	19990126	JP 1996-86324	19910830
US 5330900	A	19940719	US 1991-806928	19911212
ES 2131529	T3	19990801	ES 1992-915721	19920305
US 5639907	A	19970617	US 1992-959531	19921013
CA 2157917	AA	19940929	CA 1994-2157917	19940315
WO 9421821	A1	19940929	WO 1994-US2549	19940315
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, TT, UA, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9464449	A1	19941011	AU 1994-64449	19940315
EP 689611	A1	19960103	EP 1994-912204	19940315
EP 689611	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08507694	T2	19960820	JP 1994-521100	19940315
JP 3632856	B2	20050323		
EP 1120652	A1	20010801	EP 2001-102819	19940315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AT 212722	E	20020215	AT 1994-912204	19940315
US 5543295	A	19960806	US 1994-233085	19940425
US 5679802	A	19971021	US 1995-433996	19950504
US 5654154	A	19970805	US 1996-588260	19960118
US 5831102	A	19981103	US 1996-598353	19960208
US 5994073	A	19991130	US 1997-850009	19970501
US 5856522	A	19990105	US 1997-882330	19970625

PRIORITY APPLN. INFO.:	US 1990-574786	A3 19900830
	US 1991-806928	A2 19911212
	US 1992-959531	A2 19921013
	US 1989-367772	B3 19850515
	US 1986-889823	A1 19860724
	US 1987-140197	B2 19871231
	US 1990-559152	A2 19900725
	JP 1991-518245	A3 19910830
	EP 1992-915721	A 19920305
	US 1993-31471	A 19930315
	EP 1994-912204	A3 19940315
	WO 1994-US2549	W 19940315
	US 1994-233085	A1 19940425
	US 1995-433996	A1 19950504
	US 1996-588260	A1 19960118

OTHER SOURCE(S): MARPAT 125:269847

AB Chemiluminescent bioassays for the detection or quantitation of an analyte in a sample use 1,2-**dioxetanes** as substrates for the enzyme of an enzyme complex that binds to the analyte. The chemiluminescence obtained from the decomposition of the **dioxetane** triggered by the enzyme through the formation of the corresponding 1,2-**dioxetane** oxyanion of the enzyme complex is enhanced by the addition of TBQ [poly(vinylbenzyltributylammonium chloride)] as an enhancement agent. Other polymeric quaternary onium salts can be used as enhancement agents in conjunction with enhancement additives which improve the ability of the enhancement agent to form hydrophobic regions in the aqueous sample, in which regions the 1,2-**dioxetane** oxyanion and its chemiluminescent decomposition products can be sequestered. A kit for performing such assays is also provided.

L12 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:169405 CAPLUS
DOCUMENT NUMBER: 122:260545
TITLE: Additives for enhancing chemiluminescent assays using 1,2-**dioxetanes** as substrates
INVENTOR(S): **Bronstein, Irena Y.**; Edwards, Brooks; Voyta, John C.
PATENT ASSIGNEE(S): Tropix, Inc., USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9421821	A1	19940929	WO 1994-US2549	19940315
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, TT, UA, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ES 2131529	T3	19990801	ES 1992-915721	19920305
US 5547836	A	19960820	US 1993-31471	19930315
CA 2157917	AA	19940929	CA 1994-2157917	19940315
AU 9464449	A1	19941011	AU 1994-64449	19940315
EP 689611	A1	19960103	EP 1994-912204	19940315
EP 689611	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08507694	T2	19960820	JP 1994-521100	19940315
JP 3632856	B2	20050323		
AT 212722	E	20020215	AT 1994-912204	19940315
US 5856522	A	19990105	US 1997-882330	19970625

PRIORITY APPLN. INFO.:

US 1993-31471	A	19930315
US 1990-574786	A3	19900830
US 1991-806928	A2	19911212
EP 1992-915721	A	19920305
US 1992-959531	A2	19921013
WO 1994-US2549	W	19940315
US 1995-433996	A1	19950504

OTHER SOURCE(S): MARPAT 122:260545
AB Disclosed is additives for enhancing chemiluminescent bioassays for the presence or concentration of an analyte in a sample use 1,2-**dioxetanes** as substrates for the enzyme of an enzyme complex that bind to the analyte. The additives include surfactant (e.g. Tween 20), solvent (e.g. isopropanol, polyvinyl alc.), and water-soluble polymers (e.g. polymeric quaternary onium salts). The chemiluminescence obtained from the decomposition of the **dioxetane** triggered by the enzyme through the formation of the corresponding 1,2-**dioxetane** oxyanion of the enzyme complex is enhanced by the addition of poly(vinylbenzyltributylammonium chloride) as an enhancement agent. Other polymeric quaternary onium salts can be used as enhancement agents in conjunction with enhancement additives which improve the ability of the enhancement agent to form hydrophobic regions in the aqueous sample, in which regions the 1,2-**dioxetane** oxyanion and its chemiluminescent decomposition products can be sequestered. A kit for performing such assays is also provided.

L12 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:18074 CAPLUS
DOCUMENT NUMBER: 116:18074
TITLE: Use of organic or fluorescent enhancers in

chemiluminescence assay using acid or alkaline phosphatase and **dioxetane** substrates

INVENTOR(S): **Bronstein, Irena**; Edwards, Brooks; Voyta, John C.

PATENT ASSIGNEE(S): Tropix, Inc., USA

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03053897	A2	19910307	JP 1989-188682	19890720
JP 2984282	B2	19991129		
PRIORITY APPLN. INFO.:			JP 1989-188682	19890720

OTHER SOURCE(S): MARPAT 116:18074

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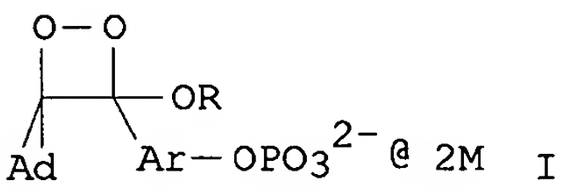

I

AB A chemiluminescence assay uses acid phosphatase on alkaline phosphatase and **dioxetane** derivs. I (Ad = adamantyl; R = lower alkyl; M = cation; Ar = aromatic) in the presence of an enhancer such as polyvinylbenzyl(benzyldimethylammonium)chloride (BDMQ). The assay can be easily measured since a high chemiluminescence d. is generated in the system. Thus, α-fetoprotein (AFP) in a sample was treated with alkaline phosphatase-anti-AFP Fab conjugate and incubated with an anti-AFP mouse IgG-coated polystyrene bead at room temperature for 20 min. The bead was washed, incubated with a substrate solution containing 3-(2'-spiroadamantane)-4-methoxy-4-(3''-phosphoryloxy)phenyl-1,2-**dioxetane** di-Na salt, BDMQ, MgCl2, ZnCl2 and pH 9.8 Tris buffer at room temperature for 20 min and the reaction mixture was counted with a luminometer for AFP determination A marked enhancement was noted compared to controls (i.e. assay system containing no BDMQ).

L12 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:651641 CAPLUS

DOCUMENT NUMBER: 115:251641

TITLE: Composition and chemiluminescent assay using a chemiluminescent compound and a hydrosoluble activator

INVENTOR(S): Voyta, John C.; Brooks, Edwards; **Bronstein, Irena Y.**

PATENT ASSIGNEE(S): Tropix, Inc., USA

SOURCE: Fr. Demande, 44 pp.
CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2649205	A1	19910104	FR 1989-8844	19890630

FR 2649205 B1 19950217
PRIORITY APPLN. INFO.: FR 1989-8844 19890630
AB A chemiluminescent assay is carried out in the presence of a substance that is sufficiently hydrosol to activate the intensity of energy liberated by the decomposition of the chemiluminescent agent. An aqueous composition comprises the decomposable chemiluminescent compound and the hydrosol. substance. TSH was determined using monoclonal anti-TSH antibody-alkaline phosphatase, Na2 3-(2'-spiroadamantane)-4-methoxy-4-(3''-phosphoryloxy)phenyl-1,2-**dioxetane**, and bovine serum albumin as the activator substance. Samples containing the albumin had a much greater luminescent intensity over samples lacking the albumin.

L12 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:578856 CAPLUS
DOCUMENT NUMBER: 115:178856
TITLE: Chemiluminescence enhancement with macromolecules and quaternary ammonium polymers
INVENTOR(S): Voyta, John C.; Brooks, Edward; **Bronstein, Irene**
PATENT ASSIGNEE(S): Tropix, Inc., USA
SOURCE: Brit. UK Pat. Appl., 46 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2233451	A1	19910109	GB 1989-14749	19890627
GB 2233451	B2	19930915		
DE 3921609	A1	19910103	DE 1989-3921609	19890630
DE 3921609	C2	19981126		

PRIORITY APPLN. INFO.: GB 1989-14749 A 19890627
AB Water-soluble enhancer substances, generally macromol. in nature, for example globular proteins such as bovine serum albumin, and polymeric quaternary ammonium salts such as poly(vinylbenzyltrimethylammonium chloride), which have the ability to inhibit non-light-emitting pathways of fluorophores are disclosed as permitting the stabilization, and hence increasing the light intensity, of such light-emitting fluorophores in aqueous media as compared to the intensity of the light emitted by the same quantities of such fluorophores in aqueous media in the absence of the enhancer substances. The enhancers may optionally be used with an auxiliary fluorophore, e.g. fluorescein. The enhanced chemiluminescent substances are preferably 1,2-**dioxetane** derivs. In immunochem. determination of TSH, the chemiluminescence of 3-(2'-spiroadamantane)-4-methoxy-4-(3''-phosphoryloxy)phenyl-1,2-**dioxetane** Na2 cleaved by alkaline phosphatase antibody conjugate, was enhanced by the addition of bovine serum albumin.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	98.07	98.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-11.68	-11.68

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